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Origin of the large p -type conductivity in the misfit layered $\text{La}_5\text{Cu}_6\text{O}_4\text{S}_7$ oxide sulfide: a first-principles study¹ ARTHUR J. FREEMAN, JINO IM, KANBER LAM, GIANCARLO TRIMARCHI, KENNETH R. POEPELMIER, Northwestern University, Evanston, Illinois — Large p -type, i.e., hole, conductivity has been achieved only in very few transparent conducting oxides. Oxide sulfides can potentially display higher hole conductivity than oxides, due to the favorable hybridization between metal and sulfur orbitals at the valence band maximum. The layered oxide sulfide LaCuOS has been identified and extensively investigated as a p -type transparent conductor, yet its layered misfit analogue $\text{La}_5\text{Cu}_6\text{O}_4\text{S}_7$ was found to have an intrinsically larger hole conductivity and an optical gap of ~ 2.0 eV. We find through first-principles density-functional calculations that the S atoms in the chains embedded in the La-O layer in $\text{La}_5\text{Cu}_6\text{O}_4\text{S}_7$ can form S_2 dimers. Absence of dimers in the S chain results in a metallic band structure. This dimerization controls the opening of an optical gap. A random distribution of S_2 dimers together with isolated atoms along these S chains is a possible mechanism for the concurrent opening of an optical gap and the presence of a significant hole concentration in this material.

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